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A Scalable Software Plan for The Undersea Warheads' Modeling and Simulation Program

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13. ABSTRACT (Maximum 200 words) The Department of Defense has embarked on an underwater explosion project to couple underwater explosion hydrodynamics with new capabilities in large deformation structural mechanics. In a related effort, DoD has recognized the urgent need of a self-consistent numerical capability for modeling explosion and shock effects in surf zone seafloor sediments with seawater and free-air pore fluid, to accelerate the progress of performance prediction of mine countermeasure efforts and for modeling the response of geometrically complex structures buried in sand or soil under blast and shock loads. This report summarizes a research plan which involves the development and implementation of a scalable, fully coupled fluid-structure interaction model for simulating the response of geometrically complex structures subjected to unsteady blast and bubble loads stemming from explosions in deep ocean and the surf zone. This multilevel, multiyear plan will couple a scalable, finite-difference hydrodynamics code for modeling the generation and evolution of propagating explosive blast waves in a medium (water, partially or fully saturated sand, "dry" soils, and sands) to a scalable, finite-element structural mechanics code for modeling the response of complex, multidimensional structures to the loads and stresses stemming from the medium.			
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A SCALABLE SOFTWARE PLAN FOR THE UNDERSEA WARHEADS' MODELING AND SIMULATION PROGRAM

EXECUTIVE SUMMARY

The research plan entails the development and implementation of a scalable, fully coupled fluid-structure interaction (FSI) model for simulating the response of geometrically complex structures subjected to unsteady blast and bubble loads stemming from explosions in the deep ocean and the surf zone (partially and fully saturated sand). This multilevel, multiyear plan will couple a scalable finite difference hydrodynamics code for modeling the generation and evolution of propagating explosive blast waves in a medium (water, partially or fully saturated sand, "dry" soils and sands) to a scalable finite element structural mechanics code for modeling the response of complex, multidimensional structures to the loads and stresses stemming from the medium. This coupled scalable model will be used to address problems of vital interest to the Department of Defense (DoD). The ultimate goal of this plan is to develop software capable of interfacing several scalable computational fluid dynamics (CFD) models with several scalable computational structural mechanics (CSM) models. As a precursor to this ultimate goal, the scalable, multiphase, FAST3D CFD code will be coupled to the scalable, LS-DYNA3D Computational Structural Mechanics (CSM) code using the Dynamic Virtual Cell Embedding (DVCE) technique as the interface.

This plan will couple the ongoing research and parallel development efforts among Navy, Army, and private industry scientists and engineers conducting large-scale hydrodynamics and structural mechanics simulations. This collaborative team will exploit existing technologies from both the hydrodynamics and structural mechanics arenas and will develop, validate, document, and demonstrate the scalable algorithms on fluid-structure interaction problems of vital interest to the Department of Defense (DoD).

The implementation of the fully coupled, scalable CFD-CSM model will result in two, somewhat overlapping, research thrusts:

- (1) a capability to compute unsteady explosive blast and bubble loads on submerged and surface vessels and the large deformation response to those loads; and
- (2) an operational simulation capability to assess explosion and shock propagation effects in the surf zone (partially saturated sand/sediment environments).

In addition, the plan has a built-in flexibility that will allow for the ability to compute unsteady blast and shock loads on complex structures fully or partially buried in varying geologies and the structural response to those loads. External loads on a structure surrounded by a medium other than air are significantly affected by the response of the medium, and the resulting structural behavior has never before been accurately predicted because of inadequacies in fully coupled media-structure interaction techniques. The benchmark calculations planned for this program will address problems of critical interest to the DoD that are not amenable to solution on current vector platforms. These demonstration calculations are designed to improve the effectiveness of weapons, enhance the survivability of undersea and surface platforms against blast and bubble loads, improve the predicted performance of mine countermeasure efforts in the surf zone, and improve the survivability/lethality of geometrically complex structures buried in varying geologies.

A SCALABLE SOFTWARE PLAN FOR THE UNDERSEA WARHEADS' MODELING AND SIMULATION PROGRAM

GOALS AND OBJECTIVES

By using this software, the goals are to develop scalable, computational simulation technology that will improve the effectiveness of weapons, enhance the survivability of undersea and surface platforms against blast and bubble loads, and enhance the performance prediction of mine countermeasure efforts in the surf zone. In addition, the flexibility of this scalable software plan will allow for a research effort focused on the clarification of lethality and survivability issues related to the structures buried in (dry) sand and soil. To achieve these goals, a scalable computational fluid dynamics (CFD) model will be coupled to a scalable computational structural mechanics (CSM) model to provide the capability to compute unsteady blast and explosive bubble loading on submerged and surface vessels and the large deformation response to those loads; to develop an operational simulation capability to assess explosion and shock propagation effects in coastal, shallow water (including partially saturated sand/sediment environments); and to compute unsteady blast and shock-loading on structures buried in sand or soil and the structural response to those loads.

The Department of Defense (DoD) has undertaken an underwater explosion (UndEx) project to couple underwater explosion hydrodynamics with new capabilities in large deformation structural mechanics. In a related effort, DoD has recognized the urgent need of a self-consistent numerical capability for modeling explosion and shock effects in surf zone seafloor sediments—primarily sands—with seawater and free-air pore fluid, to accelerate the progress of performance prediction of mine countermeasure efforts (MCM). Modeling the response of geometrically complex structures buried in sand or soil under blast and shock loads is comparable to the MCM problem where the pore water would play a minor role. All three projects are similar in the sense that they involve coupling an accurate, high-resolution hydrodynamic model with an efficient, large deformation computational structural mechanics model. The MCM and soil-structure efforts are further complicated by the need to incorporate a physics-based constitutive model for the complex medium and the associated stress terms in the conservation equations for the medium.

DESCRIPTION OF SCALABLE SOFTWARE PROJECT

This plan couples the efforts of the Naval Research Laboratory (NRL), Livermore Software Technology Corporation (LSTC), Naval Surface Warfare Center (NSWC), and the U.S. Army Engineer Waterways Experiment Station (CEWES). The NRL contribution to this effort exploits our expertise in complex-geometry CFD based on high-resolution, flux-corrected transport (FCT) algorithms, new parallel algorithms for simulating dynamic air-water interfaces, a dynamic version of the virtual cell embedding technique (DVCE) that will serve as the coupler between the hydrodynamics code (FAST3D) and structural mechanics code (LS-DYNA3D) and an elastic-plastic effective stress multimaterial hydrodynamic model for simulations of dry sands and soils and the gassy sediments in the surf zone environment. The LSTC contribution is focused on the parallelization, optimization, and coupling of LS-DYNA3D, a general purpose, explicit, three-dimensional (3-D), finite-element application used to analyze the large deformation response of inelastic solids and structures. NSWC has many years of experience with both the experimental and modeling aspects of the fluid-structure interaction problem. CEWES has extensive experience in

modeling and simulating the dynamic, nonlinear response of civilian and military structures to blast loads and in the constitutive modeling of various geological materials.

The parallel FAST3D CFD code with the virtual cell embedding (VCE) grid generator for complex geometry uses a globally structured grid. FAST3D is a compressible fluid dynamics flow solver applicable to problems such as noise generation in supersonic jets, reactive flow in ram accelerators, and low-speed flows such as the unsteady airwake over a complex Navy ship superstructure. The multiphase version of FAST3D is being used to model wave-breaking over complex geometries and underwater explosion and bubble dynamics. FAST3D was designed to be scalable since these applications require large grid sizes as well as long run times to collect unsteady flow field data. FAST3D solves the unsteady 3-D transport equations using the FCT algorithm with the VCE method for complex geometries. The FCT algorithm is a high-order, monotone, conservative, positivity preserving algorithm. In our FAST3D model, this version of the FCT algorithm solves the 3-D flow equations using a direction-split, time-split method, essentially creating a series of one-dimensional (1-D) equations that the FCT algorithm time integrates. In addition, a structured, orthogonal, rectilinear mesh is used for 3-D problems. In turn, this would require extremely fine grids for accurate solution around complex bodies; however, the VCE method circumvents this problem.

The VCE method improves the accuracy around complex bodies without sacrificing speed or memory. While the VCE method uses a structured, rectilinear grid, the cells with the VCE method may be full outside the body, fully inside the body, or partially inside the body. It is the partially obstructed cells, those cells “cut” by the surface of the body, that are given special treatment. To correctly compute the fluxes in these partially obstructed cells, the unobstructed face areas and volumes are needed. These cells are subdivided into a number of smaller subcells with which the areas and volumes can be calculated to arbitrary accuracy. Using the VCE method, only those cells next to the body are subdivided. The term “virtual” is used since the subcells embedded within a cell are not stored in memory and therefore are not integrated in the flow solution. Central processing unit (CPU) time is not sacrificed appreciably since only those cells next to the body require special treatment. The information computed from the subcells (computed once and stored) is stored in a list at the location indicated by a pointer stored in the parent cell. The division into subcells can be made so fine that the body is essentially smooth without staircasing. VCE has been shown to provide accurate results when tested on a series of 2- and 3-D problems. A dynamic version of VCE has been developed, which models moving body boundaries (motion prescribed) with a high degree of accuracy. A deformable body boundary model is undergoing development. Obviously DVCE requires that the areas and volumes be recalculated at every, or nearly every, time step. This is tantamount to developing a scalable version of the grid initializer that is under development. It is our goal to implement DVCE as the core of the interface algorithm coupling the CFD and the CSM models.

LSTC is the leading developer of the software used for the analysis of nonlinear mechanics. LSDYNA3D is a general-purpose, explicit, 3-D finite element application used to analyze the large deformation response of inelastic solids and structures. It has a full interactive graphic capability, which enables the user to monitor complex simulations. Because of its design as a general-purpose program, versatility, and relative ease of use LS-DYNA3D has become a standard in a number of application areas and industries that include automotive, aerospace, metal manufacturing, plastics, and defense. The results generated by the program have been repeatedly correlated with experimental data, thus providing confidence in computer simulations.

The program can be used on a wide range of computer architectures from workstations to supercomputers. A massively parallel version of the program has been developed recently to take advantage of the new hardware platforms that will most likely enable the solution of problems that currently cannot be run because of insufficient computing resources. Several customers are currently using the beta version of LS-DYNA3D reprogrammed to run on massively parallel systems, including the CRAY T3D, Intel Paragon, and the IBM SP2.

NSWC has been involved in both the experimental and modeling and simulation aspects of the underwater explosion fluid-structure interaction problem for a number of years. The Center has extensive experience in modeling explosives, and there is a significant amount of experimental data available with which modeling comparisons can be made. Also, for a number of years, engineers have been applying an Eulerian-Lagrangian fluid-structure interaction model (DYSMAS, developed by IABG, Germany) to the study of this problem.

TECHNICAL IMPLEMENTATION PLAN

The scalable software plan entails the development of a scalable, fully coupled structure-medium interaction model for the simulation of large deformation structural response to unsteady blast and bubble-loading stemming from underwater explosions in both deep ocean and surf zone environments. This multilevel, multiyear plan will couple a scalable finite difference hydrodynamics model (FAST3D) with a scalable finite element structural mechanics model (LS-DYNA3D) to address problems of vital interest to the DoD. The program for the outyears of this endeavor will be generalized to incorporate other hydrodynamic and structural mechanics models that have extended to parallel architectures.

The intrinsically parallel nature of the FAST3D algorithms and data structure ensures that the multimaterial version of the code can be ported with little difficulty to current state-of-the-art computers and parallel computers with different architectures. The risk for the scalable implementation of the multimaterial FAST3D hydrodynamics model is very low, as the existing code requires only refinement. This aspect of the development will be funded through other sources. The vector version of the multimaterial, elastic-plastic hydrodynamic effective stress model follows the same structure as FAST3D and, as such, the risk for the scalable implementation of this algorithm is low.

A parallel version of LS-DYNA3D has been implemented by LSTC. It requires effort to optimize domain decomposition and improve the efficiency of the contact search algorithms. The risk element in this endeavor is low.

Implementation of a scalable version of DVCE entails parallelization of the grid initializer. Only those cells next to the body require special treatment, and the information computed from the subcells is stored in a list at the location indicated by a pointer stored in the parent cell. If each processor has sufficient memory or if the body geometry is analytic (cylinders, spheres, etc), this task is trivial. With extremely complex and detailed geometries, the effort may involve judicious domain decomposition. Overall, the risk is small. Developing the coupler itself between the CFD module and the CSM module does involve some risk. We intend to minimize the risk by first coupling the vector version of FAST3D to LS-DYNA3D with DVCE as the interface using a message-passing protocol (e.g., MPI or PVM). This approach will also enhance cross-platform portability and software reusability. Development and verification of the vector form of the coupler will be funded by other sources. The risk in this aspect of the initiative is moderate.

TARGET COMPUTER SYSTEMS AND REQUIRED RESOURCES

The intent is to develop scalable software that is portable on a wide range of systems. Specific systems include Cray T3D, IBM SP-2, Intel PARAGON, and clustered workstations. For production, each individual simulation may require up to several hundred Cray C-90 equivalent hours. The 3-year estimated hours would be approximately 8000 (C-90) equivalent hours.

There is a wide range of both vector and parallel platforms available to the agencies of the DoD. Typically, requests for proposals for computer allocations on the High Performance Computing Modernization Plan (HPCMP) systems are released in August. Computer time on the HPCMP systems are allocated by using a proposal submission and review process. Typically, there is a single call for proposals for the allocations on the HPCMP systems currently available; subsequently calls for allocations on new systems may be submitted when they become available. The Appendix contains a summary listing of the resources currently available.

DEMONSTRATION CALCULATIONS AND RELEVANCE TO CRITICAL DOD CSM PROBLEMS

The demonstration calculations will directly address critical DoD structure-medium interaction problems associated with weapons effectiveness, enhanced lethality and survivability of undersea and surface platforms, improved performance prediction of mine countermeasure efforts, and improved survivability and lethality of buried structures. The latter effort is included in this plan solely for completeness. Extensive benchmark tests range from shock and bubble-loading on single- and double-walled cylinders to shock and bubble-loading on double-walled submarines, explosive shock-loading of fully or partially buried mines in the surf zone and of structures buried in sand or soil. There is an extensive database available to make detailed comparisons with experiments to ensure rapid progress and verification.

The development and implementation of a scalable, fully coupled structure-medium interaction model has significant dual-use applications. There is the potential for improved hull design for commercial vessels displaying reduced susceptibility to wave damage and reduction of cavitation-induced shafting and machinery vibration, double-hulled tanker design, earthquake-safe double-hulled storage tanks, complex geometry oceanic drag, predictions for harbor and shore-line maintenance, pier damage caused by wave action and storms, and prediction of the evolution of the benthic boundary layer in response to storms, dredging, and other man-made disturbances, to cite just a few.

SCALABLE SOFTWARE PRODUCTS & OTHER DELIVERABLES

Project deliverables and participants are listed below by year. Additional deliverables include refereed publications, progress reports, conference proceedings, and benchmark comparisons and documentations. The agencies involved in completing the tasks are also listed.

FIRST YEAR

- Implement scalable version of the multimaterial FAST3D hydrodynamic model (NRL); includes developing scalable versions of reactive burn models and tabular EoS.
- Develop scalable version of the DVCE coupler (NRL).

- Begin optimization of scalable version of the LS-DYNA3D structural mechanics model (LSTC); includes improving efficiency of contact search algorithm and modifying/optimizing domain decomposition for the noncontact case.
- Begin implementation of automated domain decomposition for the contact case (LSTC).
- Couple vector version of FAST3D to LS-DYNA3D with DVCE using a message passing protocol (e.g., MPI, PVM) (NRL, LSTC, CEWES, NSWC).
- Benchmark calculations against theoretical and experimental results.
- Benchmark all scalable models against vector versions of the same models (NRL, LSTC, CEWES, NSWC).

SECOND YEAR

- Couple scalable version of FAST3D to scalable version of LS-DYNA3D using DVCE (NRL, LSTC); includes improving efficiency of locating the wet surface.
- Incorporate scalable model of 3-D stress terms into FAST3D hydrodynamic model (NRL, CEWES).
- Optimize LS-DYNA3D to take advantage of efficient load balancing (LSTC).
- Complete benchmark tests for shock/explosion bubble loading on single- and double-walled cylinders and single walled spheres (NRL, LSTC, NSWC); including end closures on cylinders with and without internal supports.
- Begin benchmark tests for shock/explosion bubble loading on single-hulled ships and submarines (NRL, LSTC, NSWC).
- Begin benchmark tests for explosive loading of structure buried in dry soil (NRL, LSTC, CEWES).

THIRD YEAR

- Enhance completed scalable FSI model to be portable on a wide range of systems (NRL, LSTC).
- Complete above benchmark tests, if not yet completed (NRL, LSTC, NSWC).
- Perform additional benchmark tests from among:
 - shock/explosion bubble loading on a full ship hull;
 - shock/explosion bubble loading on double-hulled submarine;
 - explosive shock loading on fully or partially buried mine in the surf zone; and
 - explosive shock loading on structure buried in sand/soil (NRL, LSTC, NSWC, CEWES).
- Generalize structure-medium coupler to incorporate other hydrodynamic and structural models (NRL, LSTC, CEWES, NSWC).

SUMMARY

The goal of this scalable software plan is to develop and implement a scalable, fully coupled fluid-structure interaction (FSI) model for simulating the response of geometrically complex structures subjected to unsteady blast and bubble loads stemming from explosions in deep ocean and the surf zone (partially and fully saturated sand). This multilevel, multiyear plan will couple a scalable, finite difference hydrodynamics code for modeling the generation and evolution of propagating explosive blast waves in a medium—water, partially or fully saturated sand, "dry" soils and sands—to a scalable, finite element structural mechanics code for modeling the response of complex, multidimensional structures to the loads and stresses stemming from the medium. This coupled scalable model will be used to address problems of vital interest to the DoD. The ultimate goal of this plan is to develop scalable software that would be capable of interfacing several scalable computational fluid dynamics (CFD) models with several scalable computational structural mechanics (CSM) models. As a precursor to this ultimate goal, the scalable, multiphase FAST3D Computational Fluid Mechanics (CFD) code will be coupled to the scalable LS-DYNA3D Computational Structural Mechanics (CSM) code using the Dynamic Virtual Cell Embedding (DVCE) technique as the interface.

Two parallel computing architectures are currently popular: single-instruction, multiple data (SIMD) and multiple instruction multiple-data (MIMD). In the SIMD approach, processors perform their operations in unison under the control of a master processor. SIMD machines operate efficiently on nearest-neighbor transfer of information; however, general data exchange operations, as required for unstructured grids, are very inefficient. Special routers or precompilers have been developed in an attempt to circumvent this problem. These machines are not practical for more general types of applications where the grid topology changes every few time steps (remeshing, h-refinement, etc.). Examples of SIMD architecture with distributed memory are the Connection Machines CM-1, CM-2, and CM-200, and the MASSPAR-1.

For MIMD, processors operate independently on their data, possibly using different instructions, with coordination between the processors handled by the explicit passing of messages and synchronization hardware. Most of the algorithmic considerations designed for vector machines are applicable to many MIMD machines, since, in many current designs, each node of an MIMD system is a vector processor. The software development for MIMD machines is, in many instances, more complex than that for SIMD. The Intel series of machines—the Cray T3D, IBM SP1 and SP2, and the CM-5—are examples of MIMD architecture. In general, MIMD machines provide a more flexible computing environment because different processors can work simultaneously on different subtasks. Overall, a MIMD computer is a more general purpose computer than a SIMD computer.

Since the major component of this effort is to merge two diverse software packages, significant time and effort must be expended in coordinating the data structures of the two codes. This will prove to be especially beneficial when the basic structure is generalized to incorporate other hydrodynamic codes or structural dynamics codes. The data structure should be designed in such a manner as to facilitate check-point restarting, provide fault tolerance for very long run times, allow for changes in the number of physical nodes used in the different segments of a single simulation, and ensure that dump-restart files are compatible with other serial processors required for initializing complex geometry cases and postprocessing the simulation results. In addition, portability of the individual and complete software packages must be ensured. The final software package should be flexible enough to run on several different architectures with minimal changes.

PROJECT MANAGEMENT PLAN

The Naval Research Laboratory's Laboratory for Computational Physics and Fluid Dynamics, the Livermore Software Technology Corporation, the U.S. Army Corp of Engineers, Waterways Experiment Station, and the Naval Surface Warfare Center, White Oak, will serve as project managers to assure successful completion of this effort. There is a history of joint technological efforts between NRL and NSWC and between LSTC and NSWC. Frequent dialog among the software developers at their respective headquarters is planned and required in order to ensure progress. Project reviews and annual reports will document the progress outlined above.

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Appendix

DoD High-Performance Computing Modernization Plan Resources

System Configuration	Site	Availability	Service Unit (SU) Definition
Cray C90, 16 processors, 1 GW memory, 4 GW SSD plus 300 GB disk and 50 TB archival storage	Navy, NAVO Stennis Space Ctr., MS	Now	1 CPU hour = 3 SU's
Cray Y-MP, 8 processors, 128 MW memory, and 256 MW SSD, 120 GB disk, and 25 TB archival storage	Navy, NAVO Stennis Space Ctr., MS	Now Classified	1 CPU hour = 1 SU
Cray C90, 16 processors, 1024 MW memory, 2048 MW SSD, 256 GB disk, and access to 10 TB robotic archival storage	Army, CEWES Vicksburg, MS	Now	1 CPU hour = 3 SU's
Cray Y-MP, 8 processors, 128 MW memory, 256 MW SSD, 250 GB disk, and access to 10 TB archival storage	Army, CEWES Vicksburg, MS	Now	1 CPU hour = 1 SU
SGI Power Challenge, 96 processors, 16 GB memory, 80 GB disk storage	Army, ARL Aberdeen, MD	Now	1 CPU hour on 1 processor node = 1 SU
Cray 2, 4 processor, 256 MW memory, 100 GB disk storage	Army, ARL Aberdeen, MD	Now 40% of system available to HPCMP Classified	1 CPU hour = 1 SU
Intel Paragon XP/S, 352 processors, 32 MB memory per processor, 44 GB disk storage plus 22 GB workspace	Air Force, WPASC Dayton, OH	Now	1 wall clock hour on 1 processor node = 1 SU
CM-5E, 256 processor s, 32 GB memory 150 GB SDA, 150 GB disk, 6 TB archival storage	Navy, NRL Washington, DC	Now 40% of system available to HPCMP	1 CPU hour on 32 processor nodes = 1 SU
CM-5, 896 processors, 28 GB memory	Army, AHPCRC Minneapolis, MN	Now 50% of system available to HPCMP	1 CPU hour on 32 processor nodes = 1 SU
IBM SP2, 400 nodes, 64-1024 MB memory per node, 1-4.5 GB disk per node, 5 TB archival storage	Air Force, MHPCC Maui, HI	Now 50% of system available to HPCMP	1 CPU hour on 1 processor node = 1 SU

IBM SP2, 80 nodes, 20 GFLOPS	Air Force, MHPCC Maui, HI	Now 50% of system available to HPCMP Classified	1 CPU hour on 1 processor node = 1 SU
Cray T3D, 128 nodes, 8 GB memory, 140 GB disk storage, 1.2 TB archival storage	Air Force, EGLIN Eglin AFB, FL	Now	1 wall clock hour on 1 processor node = 1 SU
Convex Exemplar, 32 processor, 8 GB memory, 160 GB disk	Navy, NCCOSC San Diego, CA	Now	1 wall clock hour on 1 processor node = 1 SU
Intel Paragon XP/S, 336 processors, 304 nodes with 32 MB per node, 32 nodes with 128 MB per node, 130 GB disk, plus 65 GB archival storage	Navy, NCCOSC San Diego, CA	Now Classified	1 wall clock hour on 1 processor node = 1 SU

Additional system upgrades and new systems (to be determined) will be announced as available.